

# Neocedranol

<b>Inchi:</b>	InChI=1S/C15H26O/c1-9-5-6-13-14(3,4)11-7-15(9,13)8-12(16)10(11)2/h9-13,16H,5-8H2,
<b>InchiKey:</b>	AEJKOZRRMKOBQS-UYNMTERSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	CC1C(O)CC23CC1C(C)(C)C2CCC3C
<b>Mol. weight [g/mol]:</b>	222.37

## Physical Properties

Property code	Value	Unit	Source
gf	54.83	kJ/mol	Joback Method
hf	-349.96	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.466		Crippen Method
mvol	195.500	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
tb	645.34	K	Joback Method
tc	851.43	K	Joback Method
tf	397.25	K	Joback Method
vc	0.742	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.58	J/mol×K	645.34	Joback Method
cpg	621.09	J/mol×K	679.69	Joback Method
cpg	640.66	J/mol×K	714.04	Joback Method
cpg	659.50	J/mol×K	748.38	Joback Method
cpg	677.83	J/mol×K	782.73	Joback Method
cpg	695.86	J/mol×K	817.08	Joback Method
cpg	713.82	J/mol×K	851.43	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R202816&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202816&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinp:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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